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Pentacene on Ag(111): XSW experiments

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Beamline(s): X24A

Introduction: Organic/inorganic interfaces are currently under investigation due to their critical role in molecular and bioelectronic technology. Among the various materials being studied, pentacene (C22H14), a long, flat, aromatic molecule is particularly promising for electronic applications. Pentacene forms good crystals if deposited onto flat, inert surfaces, resulting in highly anisotropic transport properties. On metal surfaces, the enhanced adsorbate substrate interaction hinders diffusion and therefore the growth of continuous layers is more challenging. Since metal contacts are an essential ingredient in most electrical devices, a microscopic picture of the molecular arrangement at the interface is essential for the understanding of the charge injection mechanism in these layers. XSW experiments have been carried out to explore to which extend this microscopic information such as the molecular orientation of the molecules at the interface may be obtained.

Methods and Materials: Pentacene has been evaporated on a clean Ag(111) substrate. The photoelectron yield of mono- and multilayers has been analyzed at the standing wave condition of the Ag substrate.

Results: A typical x-ray photoelectron spectra (XPS) using a photon energy of 2637eV obtained after deposition of 6 nm pentacene is shown in Fig.1(left). The C1s and Ag3p3/2 lines have been selected for the XWS experiments. The data have been acquired with a narrow energy window of 3.5eV to obtain a good signal to noise ratio for the weak carbon signal, and the background has been determined and subtracted by shifting the analyzer energy window for ~20eV. Fig.1(right) shows the background corrected electron yield normalized for the off-Bragg condition while scanning the photon energy through the Bragg condition for back reflection. A preliminary data analysis (curves in Fig.1right) suggests a rather flat orientation of the molecules and a Pentacene-Ag distance of 0.32(3) nm. This value is smaller than expected for pure physisorption (~0.36 nm).

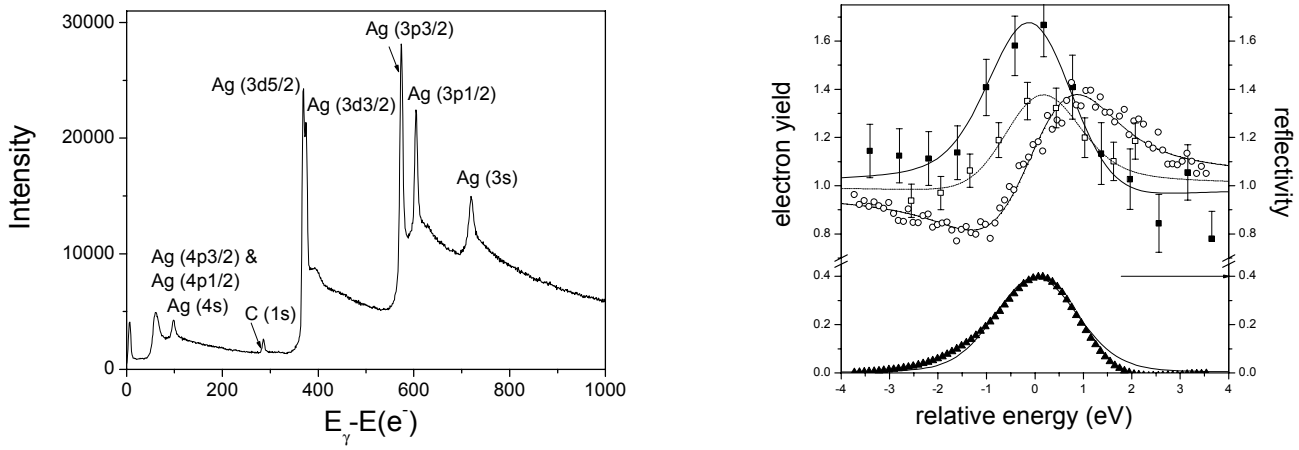

Figure1 left: Low resolution XPS data of a Ag(111) substrate covered with 6 nm Pentacene. right: X-ray standing wave data. The substrate Ag(3p3/2) electron yield is shown as open circles. The Pentacene C(1s) yield for a 60 nm overlayer is shown as open squares, while the monolayer signal obtained from annealing is shown as solid squares. The Bragg reflected intensity, normalized to the incident beam intensity, is shown as solid triangles. Lines represent least squares fits based on dynamical diffraction theory.